TITLE: Point Shifts in Rational Interpolation with Optimized Denominator

Point shifts in rational interpolation with optimized denominator

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Abstract

In previous work we have suggested obtaining rational interpolants of a function f by attaching optimally placed poles to its interpolating polynomials. For a large number of interpolation points these polynomials are well-known to be good approximants only if the nodes tend to cluster near the endpoints of the interval, as with Čebyšev or Legendre points. In practice, however, one would prefer to have them closer to equidistant. This will in particular be the case when the difficult portion of f lies well within the interior of the interval, or when approximating derivatives of f, as in the solution of differential equations. To address this difficulty, we use here a conformal change of variable to shift the points from the Čebyšev position toward a more equidistant distribution in a way that should maintain the exponential convergence when f is analytic. Numerical examples demonstrate the resulting improvement in the quality of the approximation.

1 Introduction

We are concerned here with rational approximation of a continuous function f on an interval $[a, b]$, which we may take as $[-1, 1] =: I$, after a linear change of variable when necessary. We further assume that the approximant r should interpolate f between a finite number, say $N + 1$, of distinct points (nodes) $x_0, x_1, \ldots, x_N$ in I. In a similar way as in [5], r will be constructed by attaching a certain number of poles to an interpolating polynomial.

In some applications, such as the numerical solution of two-point boundary value problems (see, e.g., [6]), one may choose the points more or less at will; in that case, one will place them so as to reach the best compromise between two often conflicting goals: points good for interpolation, on one side, and points favourable for the condition of the problem to be solved, on the other side. In [5], we have considered equidistant and Čebyšev points, the first for their regularity, the second for the condition of the interpolation and for the fast convergence of the interpolant for very smooth functions. For the solution of two-point boundary problems in [6] we have merely used Čebyšev points.

There is in general no reason besides the problem condition for accumulating the nodes toward the boundary, as with Čebyšev or Legendre points. Moreover, one of the reasons for using rational instead of polynomial interpolation is its better suitability for approximating functions with large slopes. Here too, shifting the points away from the center may not be appropriate.

Another odd consequence of accumulating interpolation points toward the extremities is the consequent ill-conditioning of the derivatives of the interpolating polynomials [7, 1]. This worsens the stability properties of time-stepping in the solution of time evolution problems with the method of lines [13] as well as the convergence of iterative methods for solving discretized stationary problems [3].

To address these difficulties, we will take advantage here of the fact that the fast convergence of the interpolant can be maintained while shifting the points with a conformal map g (independent of N) toward an equidistant position. This, however, requires an important change to the method in [5], because this point shift ruins the exponential convergence of the Čebyšev interpolating polynomial. We therefore use here as the starting interpolant the polynomial interpolating $f(g^{-1})$ in the domain of the inverse g^{-1} of the conformal map employed for the point shift, and attach poles to this polynomial.

Section 2 reviews the formulae and advantages of shifting Čebyšev points conformally toward the center of the interval when interpolating functions, and Section 3 briefly recalls the method of optimally attaching poles to the interpolating polynomial introduced in our earlier work. In Section 4 we describe how to take advantage of the better conditioning of derivatives induced by the conformal point shift; the corresponding practical improvements are finally documented with numerical examples.

2 Rational interpolation with a variable change for point shifts

Let $\mathcal{P}_m$ and $\mathcal{R}_{m,n}$, respectively, denote the linear space of all polynomials of degree at most m and the set of all rational functions with numerator in $\mathcal{P}_m$ and denominator in $\mathcal{P}_n$; furthermore, denote by f_k the interpolated values $f(x_k)$, $k = 0(1)N$, of f. Then, the unique polynomial $p \in \mathcal{P}_N$ that interpolates f at the x_k's,

$$p(x) = \sum_{k=0}^{N} f_k L_k(x), \qquad L_k(x) := \prod_{i\neq k}(x - x_i) \Big/ \prod_{i\neq k}(x_k - x_i),$$

can be written in its *barycentric form* [9]

$$p(x) = \sum_{k=0}^{N} \frac{w_k}{x - x_k} f_k \Big/ \sum_{k=0}^{N} \frac{w_k}{x - x_k}, \tag{2.1}$$

where the so–called *weight* w_k corresponding to the point x_k is given by

$$w_k := 1 \Big/ \prod_{i=0,\ i\neq k}^{N} (x_k - x_i).$$

Despite its appearance, (2.1) determines a polynomial of degree at most N: the w_k are precisely the numbers which guarantee this [4]. By choosing other w_k's, a rational interpolant is constructed.

The barycentric formula has several advantages over other representations of the interpolating polynomial ([4] p. 357). One of them is the fact that the weights appear in both the numerator and the denominator, so that they can be divided by any common factor. For example, simplified weights for Čebyšev points of the first kind $x_k^{(1)} := \cos\phi_k$, where $\phi_k := \frac{2k+1}{2(n+1)}\pi$ and $k = 0, \ldots, N$, are given by $w_k^{(1)} = (-1)^k \sin\phi_k$ ([9] p. 249), while for the Čebyšev points of the second kind $x_k^{(2)} := \cos k\frac{\pi}{N}$ – which will be used here – one simply has Salzer's formula ([9] p. 252)

$$w_k^{(2)} = (-1)^k \delta_k, \qquad \delta_k = \begin{cases} 1/2, & k = 0 \text{ or } k = N, \\ 1, & \text{otherwise.} \end{cases}$$

These points are, together with Legendre's, the most used nodes for global polynomial interpolation and large N. They achieve exponential convergence of p toward f if the latter is analytic in an ellipse E_ρ with foci at ± 1 and sum of its axes equal to 2ρ, $\rho > 1$. However, this fast convergence comes at the cost of a concentration of the nodes in the vicinity of the extremities of I. As mentioned above, this accumulation may have drawbacks, such as poor spreading of the information about f over the interval and ill-conditioning of the derivatives near the endpoints.

With a suitable choice of the interpolant, one may conformally shift the nodes toward an equidistant position (though not all the way) without losing the exponential convergence. For that purpose, one considers, beside the x-space in which f is to be approximated, another space, denoted by y, say, and the $N+1$ Čebyšev points of the second kind

$$y_k = x_k^{(2)}$$

in the interval $J := [-1, 1]$ in this y-space. Let g be a conformal map from a domain $\mathcal{D}_1$ containing J (in the y-space) to a domain $\mathcal{D}_2$ containing I (in the x-space); moreover, suppose that f is a function $\mathcal{D}_2 \mapsto \mathbb{C}$ such that the composition $f \circ g : \mathcal{D}_1 \mapsto \mathbb{C}$ is analytic in an ellipse E_ρ, as defined above. With this map we may define new interpolation points on I, $x_k = g(y_k)$, as well as the conformal transplantation $F(y) := f(x)$ [10] of f into the y-space.

Then, with the polynomial interpolating $F(y)$ at the y_k

$$A_N(y) := \sum_{k=0}^{N} F(y_k) L_k(y) = \sum_{k=0}^{N} f(x_k) L_k\big(g^{-1}(x)\big) =: a_N(x), \tag{2.2}$$

one has

$$|a_N(x) - f(x)| = \mathcal{O}(\rho^{-N}), \qquad x \in [-1, 1].$$

Rational interpolation with all poles prescribed is very simple in the barycentric setting [5]: the P poles z_i are attached to (2.1) by replacing w_k with

$$b_k = w_k d_k, \qquad d_k := \prod_{i=1}^{P} (x_k - z_i).$$

If $N \geq P$ this results in a rational interpolant in $\mathcal{R}_{N,P}$ with poles at z_i, $i = 1, \ldots, P$ (when such an interpolant exists, see [5]).

Remark 2.1 *Exponential convergence of interpolation at the shifted points is also attained with the rational function given by (2.1) with $w_k = w_k^{(2)}$ [2]. However, this is in general a rational function in $\mathcal{R}_{N,\nu}$, $\nu > N - P$: there is not enough defect in the denominator degree for the weights $w_k^{(2)} d_k$ to warrant the presence of the P poles z_i.*

We then use a_N as the starting interpolant to which we attach the poles v_i in the y-space. This yields

$$R(y) := \frac{\displaystyle\sum_{k=0}^{N} \frac{w_k \prod_{i=1}^{P}(y_k - v_i)}{y - y_k} f_k}{\displaystyle\sum_{k=0}^{N} \frac{w_k \prod_{i=1}^{P}(y_k - v_i)}{y - y_k}} = \frac{\displaystyle\sum_{k=0}^{N} \frac{w_k \prod_{i=1}^{P}\left(g^{-1}(x_k) - g^{-1}(z_i)\right)}{g^{-1}(x) - g^{-1}(x_k)} f_k}{\displaystyle\sum_{k=0}^{N} \frac{w_k \prod_{i=1}^{P}\left(g^{-1}(x_k) - g^{-1}(z_i)\right)}{g^{-1}(x) - g^{-1}(x_k)}} =: r(x).$$

If a rational interpolant with these poles exists, it is given in the y-space by R, and r is a rational function in the argument $g^{-1}(x)$. Its poles are at $z_i = g(v_i)$.

3 Construction of the optimal interpolant

Our method consists in optimizing the position of the v_i's so as to minimize

$$\|R - F\|_\infty = \|r - f\|_\infty,$$

as described in §3 of [5]. Optimal v_i's always exist, but these are not unique in general. Whether the optimal R is unique is an open question; however, for every optimized pole v_i an indicator may be calculated which, if nonzero, guarantees that v_i is indeed a pole of R.

In the practical computations documented in §5 the optimization of the v_i's was performed using the same two algorithms as in [5]: for small N we used a discrete differential correction algorithm according to [11], while for larger N the simulated annealing method of [8] was applied. Both methods will in principle locate a desired global maximum. The first method achieves it in a systematic and guaranteed way evaluating the error not continuously but on a fine grid; the simulated annealing method cannot be guaranteed to find the global extremum but, when used for an extensive search, will produce a reasonable approximation of it.

As mentioned in [5], our way of attaching poles to the interpolating polynomial has a very nice property: the approximation error can only decrease or at worst stay constant with a growing number of poles, this in sharp contrast with classical rational interpolation; when a new unknown, say v_j, is added to the set of variables, $\{v_1, \ldots, v_{j-1}\}$, the optimal values of the latter are a feasible vector for the higher dimensional optimization.

Let us conclude this section with a comment on the use of the nomenclature "attaching the poles". In classical rational interpolation, the poles of the interpolant are determined by the data. There too, however, one sometimes wishes to prescribe the location of the poles (with corresponding decrease of the number of degrees of freedom): many authors then speak of "assigning", or "prescribing" the poles. In that sense one cannot "assign" poles to a polynomial, which obviously cannot have poles. We thus start with the interpolating polynomial and its poles at infinity and make it a rational interpolant by bringing the poles into an optimal position in $\mathbb{C}$. We call this procedure "attaching poles", to distinguish it from the process of forcing a rational function to have a pole at a particular place.

4 Derivatives of the optimal interpolant with shifted points

As mentioned in §1, one of the reasons for shifting the points from their Čebyšev position toward the interior of the interval is the improvement of the condition of the derivatives resulting from such a shift. Besides r, we will evaluate also r' and r'' as approximants of f', resp. f'', and estimate $\|r - f'\|_\infty$ and $\|r - f''\|_\infty$.

Schneider and Werner [14] have noticed that every rational interpolant $R \in \mathcal{R}_{N,N}$, written in its barycentric form

$$R(y) = \sum_{k=0}^{N} \frac{u_k}{y - y_k} f_k \Bigg/ \sum_{k=0}^{N} \frac{u_k}{y - y_k},$$

can easily be differentiated. The formulae for the first two derivatives read

$$R'(y) = \begin{cases} \displaystyle\sum_{k=0}^{N} \frac{u_k}{y - y_k} R[y, y_k] \Bigg/ \sum_{k=0}^{N} \frac{u_k}{y - y_k}, & y \neq y_i, \ i = 0(1)N, \\ \displaystyle -\Big(\sum_{\substack{k=0 \\ k \neq i}}^{N} u_k R[y_i, y_k] \Big) \Big/ u_i, & y = y_i \end{cases}$$

and

$$R''(y) = \begin{cases} \displaystyle 2\sum_{k=0}^{N} \frac{u_k}{y - y_k} R[y, y, y_k] \Bigg/ \sum_{k=0}^{N} \frac{u_k}{y - y_k}, & y \neq y_i, \ i = 0(1)N, \\ \displaystyle -2\Big(\sum_{\substack{k=0 \\ k \neq i}}^{N} u_k R[y_i, y_i, y_k] \Big) \Big/ u_i, & y = y_i, \end{cases}$$

with $R[z, z, y_k] = \frac{R'(z) - R[z, y_k]}{z - y_k}$. The chain rule then yields, for $r(x) = R\big(g^{-1}(x)\big)$,

$$r'(x) = R'(y) \cdot \left[g^{-1}(x)\right]' = \frac{R'(y)}{g'(y)}, \qquad r''(x) = \frac{1}{[g'(y)]^2} R''(y) - \frac{g''(y)}{[g'(y)]^3} R'(y). \tag{4.1}$$

Specifically, in our calculations we have used the map suggested by Kosloff and Tal-Ezer [12],

$$g(y) = \frac{\arcsin(\alpha y)}{\arcsin \alpha}, \qquad 0 < \alpha < 1.$$

α	$P=0$	$P=2$	$P=4$	$P=6$	$P=8$
0.0	6.37e − 5	1.42e − 6	5.83e − 8	9.38e − 9	1.30e − 9
0.5	3.11e − 5	6.69e − 7	2.48e − 8	4.21e − 9	4.23e − 10
0.75	8.06e − 6	1.60e − 7	5.50e − 9	9.47e − 10	1.27e − 10
0.9	1.12e − 6	1.97e − 8	5.90e − 10	3.94e − 11	2.05e − 11
0.95	2.78e − 7	4.47e − 9	1.29e − 10	1.36e − 11	3.82e − 12
0.96	1.85e − 7	2.93e − 9	8.27e − 11	4.20e − 12	3.88e − 12

TAB. 1. Errors when approximating f with increasing P and α in Example 1.

In the limiting cases, $\alpha \to 0$ keeps the points at their Čebyšev position, whereas $\alpha \to 1$ renders them equidistant. The derivatives of g are given by

$$g'(y) = \frac{\alpha}{\arcsin \alpha} \frac{1}{\sqrt{1-(\alpha y)^2}}, \qquad g''(y) = \frac{\alpha^3}{\arcsin \alpha} \frac{y}{\sqrt{\left(1-(\alpha y)^2\right)^3}},$$

so that in (4.1)

$$\frac{g''(y)}{[g'(y)]^3} = (\arcsin^2 \alpha) y.$$

5 Numerical evidence

We now report on practical computations, performed on two examples, which demonstrate the efficiency of point shifts for improving the rational interpolants with optimized denominators. These examples share the property that the difficult part of f lies in the center of I, so that the shift of the points toward a more equidistant position naturally improves the quality of the information provided to the interpolation method.

α	$P=0$	$P=2$	$P=4$	$P=6$	$P=8$
0.0	5.27e − 3	1.26e − 3	4.85e − 6	8.69e − 7	1.40e − 7
0.5	2.67e − 3	5.87e − 4	2.33e − 6	4.03e − 7	4.63e − 8
0.75	7.47e − 4	1.49e − 5	5.16e − 7	9.44e − 8	1.30e − 8
0.9	1.14e − 4	2.01e − 6	6.56e − 8	4.28e − 9	2.16e − 9
0.95	2.97e − 5	4.99e − 7	1.48e − 8	1.59e − 9	4.52e − 10
0.96	2.01e − 5	3.24e − 7	9.52e − 9	4.80e − 10	4.70e − 10

TAB. 2. Errors when approximating f' with increasing P and α in Example 1.

The sup-norm $\| \quad \|_\infty$ has thereby been estimated by considering the 1000 equally spaced points $\widehat{x}_\ell = -\frac{5}{4} + \frac{\ell-1}{999}\frac{10}{4}$, $\ell = 1(1)1000$, on the interval $[-5/4, 5/4]$ and computing the maximal absolute value of the error at those $\widehat{x}_\ell$ lying in $[-1, 1]$.

Example 5.1 We have first revisited Example 3 of [5], which displays in the center of

I a slope increasing with a positive parameter, here denoted by ϵ,

$$f(x) = \cos \pi x + \frac{\mathrm{erf}(\delta x)}{\mathrm{erf}(\delta)}, \qquad \delta = \sqrt{.5\epsilon},$$

where erf denotes the error function (see [5] for a graph).

In Table 1 we give the results obtained with $\epsilon = 500$ and $N = 81$, increasing numbers P of poles and increasing α. Tables 2 and 3 display the same information for the approximation of f' and f'' with r' and r'' as given by the formulae (4.1). The combination of extra poles and a point shift brings about 7 digits of accuracy, where the point shift alone makes only for 2–3. The improvement in the derivatives is especially remarkable: the error in the second derivative decreases from the useless value of 9.26 to about 10^{-7}!

α	$P=0$	$P=2$	$P=4$	$P=6$	$P=8$
0.0	9.26	4.05e − 2	4.82e − 4	7.85e − 5	1.46e − 5
0.5	4.26	2.07e − 2	2.18e − 4	3.75e − 5	4.91e − 6
0.75	9.50e − 1	5.48e − 3	6.25e − 5	9.53e − 6	1.26e − 6
0.9	9.30e − 2	6.49e − 4	8.86e − 6	4.93e − 7	2.34e − 7
0.95	1.59e − 2	1.23e − 4	1.88e − 6	1.75e − 7	5.31e − 8
0.96	9.18e − 3	7.36e − 5	1.29e − 6	6.00e − 8	5.57e − 8

TAB. 3. Errors when approximating f'' with increasing P and α in Example 1.

Example 5.2 Example 3 in [5] has demonstrated that the attachment of poles may be very effective in improving the approximation of oscillatory functions. Here we change the function to

$$h(x) = e^{-ax^2} \sin bx, \qquad a > 0,\ b > 0,$$

so that the most oscillatory part lies in the center of the interval.

Results with $a = 5$, $b = 25$, $N = 31$, $P = 0$ and $P = 2$ are given in Table 4. In contrast with the preceding example, here the point shift brings much more improvement than the attachment of poles, about 6–7 digits, an especially heartening fact for the derivatives, to which the interpolants without shift are useless approximants.

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α	h		h'		h''	
	$P=0$	$P=2$	$P=0$	$P=2$	$P=0$	$P=2$
0.0	4.12e − 2	2.49e − 3	2.03	1.36e − 1	1.43e + 3	9.51e + 1
0.5	1.66e − 2	8.68e − 4	8.90e − 1	6.08e − 2	5.63e + 2	3.84e + 1
0.75	1.97e − 3	7.95e − 5	1.17e − 1	7.73e − 3	5.98e + 1	3.98
0.9	1.91e − 5	4.20e − 7	1.09e − 3	4.56e − 5	3.97e − 1	1.68e − 2
0.92	4.57e − 6	7.78e − 8	2.48e − 4	8.20e − 6	8.24e − 2	2.75e − 3
0.94	6.56e − 7	7.18e − 9	3.26e − 5	5.69e − 7	9.56e − 3	1.66e − 4
0.96	3.03e − 8	2.39e − 9	1.81e − 6	5.49e − 7	4.71e − 4	1.62e − 4

TAB. 4. Change in the errors induced by the introduction of two poles in Example 2.

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